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STUDY OF THE COLLISIONS OF METASTABLE ATOMS OF $He/2^3S/$ WITH HELIUM AND NEON, AND OF Ne^+ IONS WITH HELIUM

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16. Abstract A study was made of the differential scattering of beams of He*/2^3S/ and Ne* in He and Ne. The experimental functions for the systems He*-He and Ne+-He are compared with functions calculated from potentials given in the literature. Deviations are found between the calculated and the measured curves. This deviation is eliminated for the system He*-He by modifying the trend of the adiabatic term $^3\Sigma_g^+$. Functions of the potential energies of interaction corresponding to the adiabatic term $^3\Sigma_g^+$ of the system He_2^* and to the term $^3\Sigma$ of the system He*-Ne are found. An analytical approximation of the potentials found is proposed.

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STUDY OF THE COLLISIONS OF METASTABLE ATOMS OF $He/2^3S/$ WITH HELIUM AND NEON, AND OF Ne^+ IONS WITH HELIUM

A. P. Kalinin and V. B. Leonas /3*

1. In recent years the investigation of collisions of metastable He atoms with atoms of the noble gases has attracted a large number of researchers. This is due, on the one hand, to the important role of these collisions in processes in discharge and ionospheric plasmas; on the other hand, these systems are of high interest to the theory of atomic collisions, since the relative simplicity of the electronic structure opens up an approach to nonempirical calculations of their energies and thus, to quantitative predictions of effects accompanying collisions.

This present study deals with the interaction of metastable He atoms in the 2^3S state with helium and neon atoms in the free state ^1S and aims at determining the trend of molecular terms of these systems in the region of small distances of approach (most of the preceding experimental studies were concerned with the interaction at large distances [1]).

In the case of the system $He^*/2^3S/$ - $He/1^1S/$ symmetry leads to the initiation of two terms -- even $/^3\Sigma_g^+/$ and odd $/^3\Sigma_u^+/$ (Fig. 1), and the scattering pattern is the effective superpositioning of the contributions of both states. Methodological capabilities of the present experiment do not permit the extraction of information on the trend of individual terms from the observable scattering pattern and therefore in the case of the system $He^*/2^3S/$ - $He/1^1S/$ the aim was to find the degree of accuracy of the most reliable nonempirical calculations [2] /4

* Numbers in the margin indicate pagination in the foreign text.

of the terms $^3\Sigma_{u,g}$ based on a comparison of predictions from these calculated and measured scattering patterns.

~~In the case~~ of the system He*-Ne, the goal was to determine the trend of the $^3\Sigma$ term and to find the nature of its approximation toward the cut-off of the continuous spectrum corresponding to the lowest terms $^2\Sigma$ and $^2\Pi$ of the molecular ion $/HeNe/^+$ calculated in [3]. To verify the accuracy of these calculations, an additional study was made of the scattering of a beam of Ne^+ ions in helium and the pattern observed was comparedwwith the pattern calculated on the basis of the theoretical potentials given in the paper [3]. The poor agreement found indicates the necessity of refining the energy calculations of the system $/HeNe/^+$.

II. A study of the scattering of a beam of $He^*/2^3S/$ with energies E = 400, 600, 1200, and 2000 eV at small angles was conducted on a stand shown in Fig. 2. Here: 1 is a Nirovskiy-type ion source; 2 is a magnetic mass analyzer emitting ions with the necessary mass; 3 is a charge-exchange chamber for obtaining neutral particles from ions; 4 is a deflecting capacitor in which the noncharge-exchanging ions are removed from the primary beam; 5 is a scattering chamber with electromagnetic valve 6 with which the scattering gas can be released alternately into the scattering chamber or into the vacuum vessel; 7 is a detector, which is shifted along an arc relative to the center of the scattering chamber within the range of angles $\alpha = 1 \cdot 10^{-3}$ to $4 \cdot 10^{-2}$ rad. The charge-exchange chamber is an oven with controllable wall temperature and thus, in addition to the gas targets, the vapor of alkali metals can be used for charge-exchange purposes.

A channel-type electronic multiplier (CEM) was used as the particle detector; the CEM significantly improved the resolving /5 power of the recording of scattered particles through a reduction of the dimensions of the slits of the scattering chamber and the detector. The recording was carried out in the discrete recording mode. It should be noted that the efficiency of recording metastable particles at the beam energies used was close to unity, while the efficiency of recording atoms deactivated to the ground state at the energy of 600 eV will become equal to 0.8 [4] and this circumstance must be taken into account when interpreting the experimental data. In the study of the scattering of Ne^+ in He, the use of the deflecting capacitor made it possible to measure the differential scattering of ions and to preclude the effect of charge exchange. For He*-He, the flux measured by the detector included both elastically scattered particles, as well as particles scattered with transfer of excitation.

The entrance slit of the scattering chamber determining beam geometry was an opening with a diameter of 0.1 mm. The distance from the center of the scattering chamber to the detector was 212 mm. A diaphragm with an opening of 0.3 mm was placed in front of the CEM entrance.

A calibration technique was used to determine the absolute values of the differential cross-sections. Essentially, the technique amounted to measuring, at the same gas pressure in the scattering chamber, the flux of scattering particles for both the system under study and the system whose absolute differential cross-section is known or can be calculated on the basis of available reliable interaction potential data. This avoided the necessity of measuring the pressure in the scattering chamber.

To obtain a beam of He*/2^3S/ atoms, use was made of quasi-resonant charge-exchange of He* ions in sodium vapor. Charge-exchange in the vapor of alkali metals is a convenient and effective way of obtaining metastable atoms [5], however in the available studies on the determination of the total charge-exchange [6] cross-sections there is no information on the population of states in the beam of charge-exchanging particles.

This estimate can be made on the basis of theoretical calculations of the partial cross-sections of charge-exchange in different states given the condition of their adequate reliability. Fig. 3 presents the results of calculations [6] of the partial cross-sections for the charge-exchange of He^+ in Na vapor. From the relative trend of the partial cross-section functions (the accuracy of their determination should be regarded as identical) it can be concluded thatt for the beam of He^+ with $E \leqslant 10^3$ eV, charge-exchange in sodium will lead to the predominant population of the 2^3S level. The admixture of the 2^1S state neglected in the case of Na, as seen from these calculations, reaches about 50 percent for charge-exchange in Cs vapor and this factor casts doubt on the homogeneity of the beams obtained by charge-exchange in Cs.

In the paper [7] use was made specifically of Cs, and one of the arguments for using Cs was the calculations made by Olson [8]. The reliability of the latter in our view is altogether inadequate for the conclusions drawn in [7] concerning beam composition.

The quantity measured in the present experiments is the current of scattered particles captured by the detector, deflected by the angle α relative to the beam axis. The level of this current was defined as the difference of the currents I_M and I_P ($I(\alpha) = I_M - \lambda I_P$), corresponding to the successive releases of the target gas into the scattering chamber and (with constant mass volume flow) -- the working volume (the value of λ here is equal to the ratio of I_M to I_P for the detector position $\alpha = 0$). The current $I(\alpha)$ can be associated with the differential scattering cross-section on the basis of involving ahcharacteristic such as the efficiency of detector collection of the scattered particles.

The collection efficiency or the apparatus function $F_\alpha(\theta)$, whose numerical determination procedure is described in detail in [9], enables us to write the following obvious relation:

$$I(\alpha) = B \int_{\Delta} \sigma(\theta, E) F_{\alpha}(\theta) \sin\theta \, d\theta \quad (1)$$ /7

Here: $\sigma(\theta, E)$ is the differential cross-section for scattering in the laboratory system of coordinates, and B is a known constant [9]. Eq. (1) is the basis for a quantitative comparison of the measured currents with the currents calculated from the differential cross-section $\sigma(\theta, E)$, which in turn is uniquely determined by the nature of the interaction (by the potential $V(r)$) of the colliding atoms. A typical appearance of the apparatus functions calculated for the geometrical conditions of the present study is shown in Fig. 4 (the arrows denote the angular positions of the detector axis α).

III. Now let us examine the main relations used in the calculation of the differential scattering cross-sections.

The complex nature of the terms of interaction of the systems studied led to the necessity of using a quantum treatment of scattering, according to which the cross-section in the center-of-mass system $\sigma(\chi)$ is associated with the scattering amplitude $f(\chi)$, which in turn is the summation of the partial waves:

$$\sigma(\chi) = |f(\chi)|^2, \quad f(\chi) = (2ik)^{-1} \sum_{\ell=1}^{\infty} (2\ell+1)[\exp(2i\eta_\ell) - 1] P_\ell(\cos\chi) \quad (2)$$

Here the symbols are the usual ones and coincide with those adopted in [10]. To compute the phases η_1 use was made of the high-energy approximation ($V(r) \ll E$), in accordance with which

$$\eta_\ell = -\frac{k}{2} \int_{\ell/k}^{\infty} \frac{V}{E} [1 - \ell/kr]^{-1/2} dr . \quad (3)$$

And in computing the integral (3), use was made of its approximation with the fast-converging series given in [11]. Use of the approximation bypassed the necessity of an analytical specification of V(R) over the entire interval of approach states used. For $\ell < \ell_{cr}$ determined from the relation $V(\ell_{cr}/k) \approx E$ calculated according to [3] the phases are deliberately incorrect; however /8
the smallness of the contribution to the sum of the partial waves

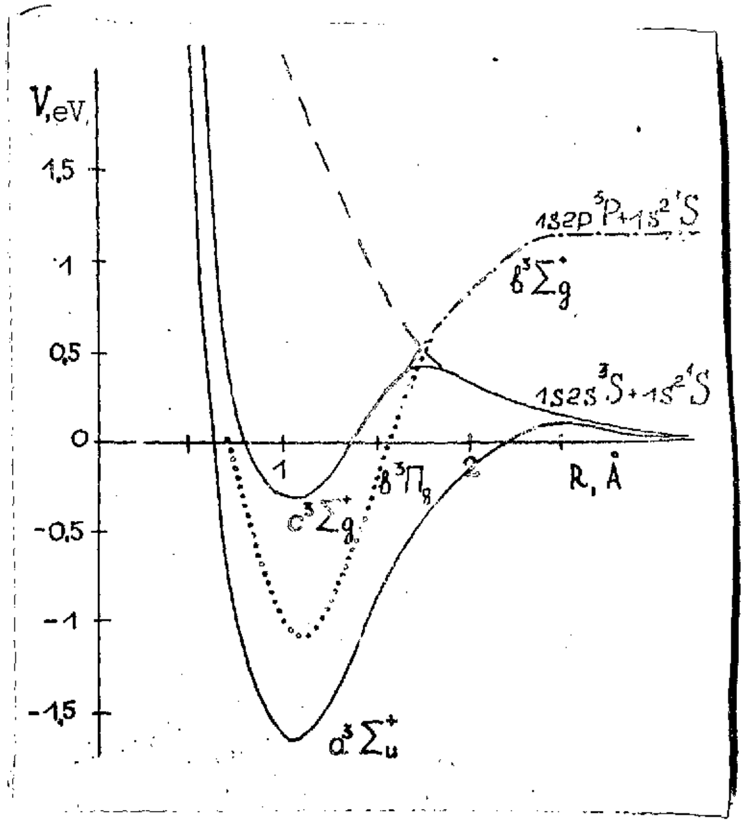

Fig. 1. Potential curves of interaction of helium atoms in various states [2]

of terms with $\ell < \ell_{cr}$ (in this case the larger values of η_l make it possible to use the approximation of the random phases) ensured the good accuracy of the approximation. The interaction for the systems He*-He and Ne^+-He is characterized by the presence of two terms that are degenerate for large n. According to [10], for He*-He the total differential cross-section of scattering σ_Π is equal to the sum of the differential cross-sections for elastic scattering σ_y and the excitation-exchange σ_o and can be written as (neglecting the contribution made by amplitudes for the angles $\sigma_I(x)$

$$\sigma_\Pi(x) = \sigma_y(x) + \sigma_o(x) = \frac{1}{4}|f_u(x) - f_g(x)|^2 + \frac{1}{4}|f_u(x) + f_g(x)|^2 = \frac{1}{2}|f_u(x)|^2 + \frac{1}{2}|f_g(x)|^2, \qquad (4)$$

where f_u and f_g are the scattering amplitudes in the $V_{u,g}$ potentials.

The differential scattering cross-section of the Ne^+ ions in He due to the absence of interference can be represented as

$$\sigma(x) = \frac{1}{3}\sigma_{\Sigma}(x) + \frac{2}{3}\sigma_\Pi(x) . \qquad (5)$$

Eqs. (4) and (5) were used in the calculations of I(α) based on [1].

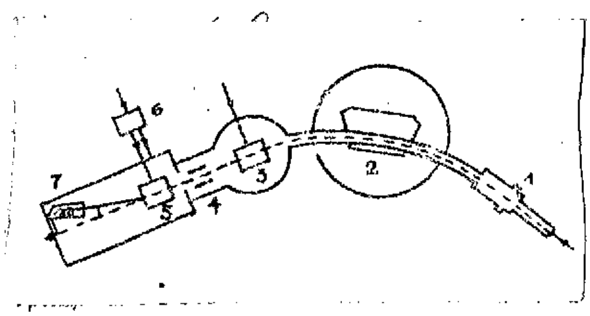

Fig. 2. Scheme of experimental setup (see text for symbols)

IV. Fig. 5, 6, and 7 present in reduced coordinates R ($I(\alpha)\,\alpha^2$) and T (αE) (equivalent to the usual functions $\int \sigma(\theta)\sin\theta \cdot \theta$ and $\tau = \theta E$) with solid lines the experimental functions for the systems He*-He, He*-Ne, and Ne^+-He for all the beam energies used. The precision of the measurements is indicated by the vertical stroke marks (each of the measured curves was measured not fewer than three times); thus, these curves yield a trend based on averaged values of the currents $I(\alpha)$. Included with this primary experimental data is a comparison of the calculated currents; the discussion of the comparison is given below.

<u>He*-He system</u>. For the calculations of the total differential scattering cross-sections, use was made of the interaction potentials shown in Fig. 1 with a solid line and calculated in [2]. A comparison of the reduced current k calculated on the /9 basis of these potentials (dashed line) with the measured values is given in Fig. 5a. As can be seen from the figure, over the entire interval of T values, a strong difference between the calculated and measured currents can be observed. Presented in this same figure, with a dashed-dot line are the results of calculating the current for the even and odd terms $^1\Sigma_u^+$ and $^1\Sigma_g^+$ corresponding to the system He/2^1S/ - He/1^1S/, using the data on the terms from [12] and [13]. The analogous difference observed precludes the possiblity of accounting for this discrepancy by the inhomogeneity of beam composition. This discrepancy cannot be explained either by the effect of perturbations caused by the inelastic channel associated with the interaction $^3\Sigma_g^+$ (or $^1\Sigma_g^+$) -term with $^3\Pi_g$ (or $^4\Pi_g$) -term corresponding to the interaction of the

$He/2^3P$, $^1P/$ - $He/1^1S/$ atoms. Allowing for this channel can only increase the discrepancy between the calculated and the measured vaue values of R in the region $T > 4.8$. The characteristic trend of $^3\Sigma_g^+$ of the adiabatic term is caused by the growing approach (non-intersection) of the terms corresponding to different $/^3P, ^3S/$ excited states of the helium atom.

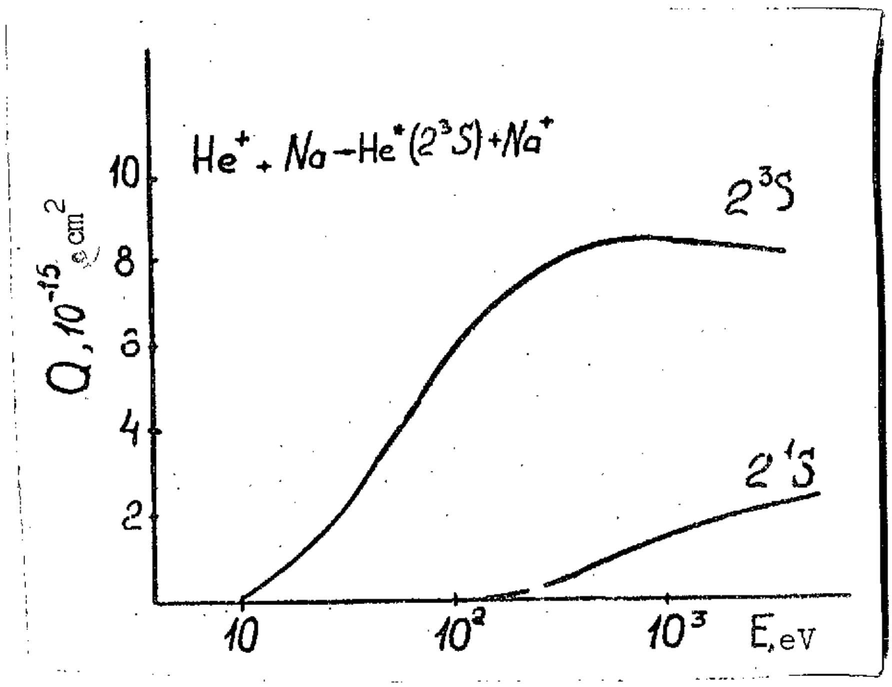

Fig. 3. Dependence of charge-exchange cross-sections of He ions in Na, according to [6]

In [14] it is concluded that the interaction of these terms leads to their very strong mutual repulsion (greater splitting at the point of approach) and a correspondingly lower probabilities of transition from one adiabatic curve to another. This result is purely theoretical and its justification can be shown only by direct experiment. These measurements also point to the converse situation. They can be quantitatively explained only on the basis of the assumption of the high (~ 1) transition probability, that is, on the basis of bringing into the calculation of scattering the adiabatic trend of the $^3\Sigma_g^+$ term. The selection of the diabatic V_g potential yielding the best agreement of the measured and calculated currents (Fig. 5 b, circles) leads to the curve shown in Fig. 1 with a dashed line and closely approximated by the function $V_g(r) = 4/r^{3.36}$ (where r is in Å, and V is in eV).

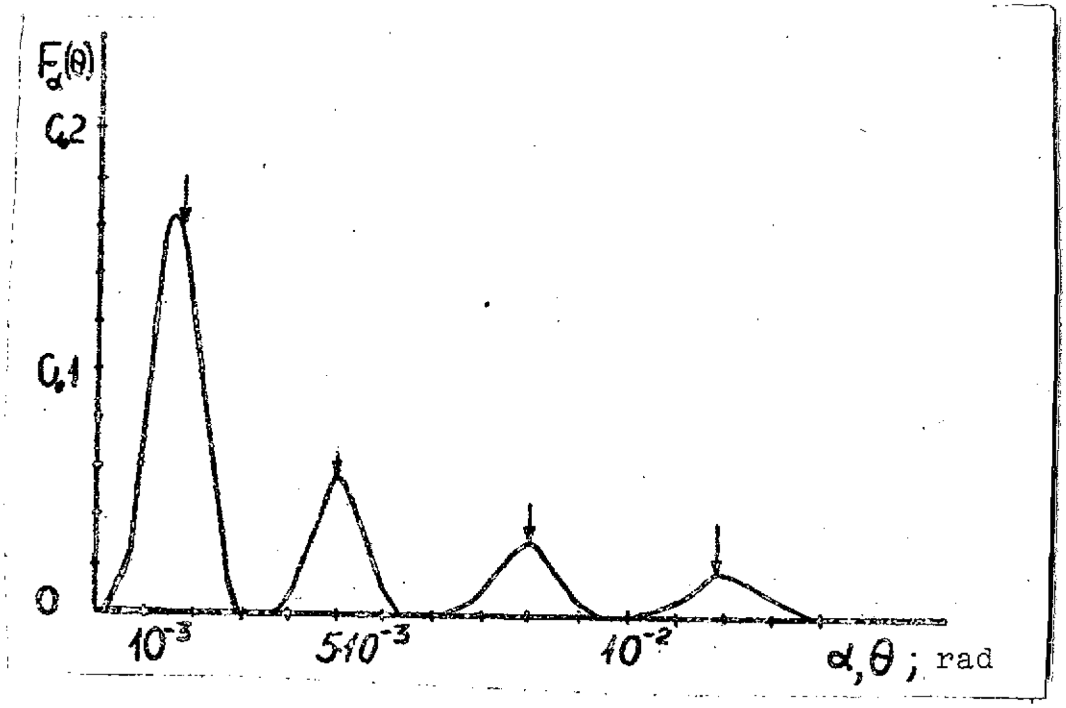

Fig. 4. Apparatus functions $F_\alpha(\theta)$ for different positions of detector α indicated by arrows

The agreement achieved here can be regarded as good, though it /10 should be noted that the measured curves are more monotonic than the calculated curves (the latter preserve traces of oscillations in the cross-sections). It can be assumed that a fuller agreement of measurements and calculations will be achieved on the basis of a calculation within the frame of reference of the approach of three states ($a^3\Sigma_u^+$, $c^3\Sigma_g^+$, and $b^3\Sigma_g$ or in $b^3\Pi_g$ /; however, these calculations are justified only when there is a substantial improvement in the resolution of the measurements of $I(\alpha)$.

He*-Ne system. The closeness of the cutoff of the continuous spectrum for the system He*-Ne opens up a theoretical possiblity of observing the perturbations of the elastic scattering pattern by transitions with the loss of an electron. The contribution made by the perturbing channel was assumed by us to be detectable upon converting the primary data $I(\alpha)$ into $\sigma(\theta, E)$. In the event of the smallness of the contribution made in the reduced

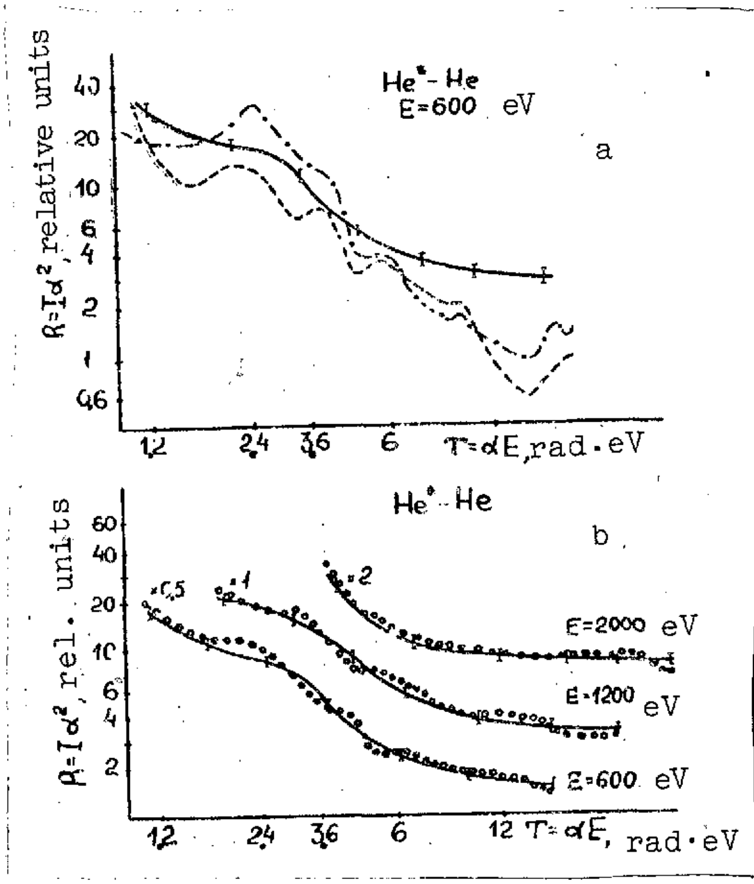

Fig. 5. Comparison of experimental and calculated functions R(T) (see text for symbols)

a. for theoretical potentials [2, 12, 13]

b. for the empirically found trend of the $^3\Pi_g$ term

coordinates ρ and τ, the measurements must fit on a single curve. This single curve was actually obtained for measurements with energies E = 400, 600, 1200, and 2000 eV (Fig. 6b) and therefore it can be assumed that within the limits of measurement error, the perturbing effect of the continuous spectrum is absent. For single-channel (elastic) scattering, Eqs. (2) and (3) give a method of calculating the cross-section based on the assumed potential V(r). Precisely by varying the trend of the tabulated V(r), the agreement of the measured and the calculated functions R(t) shown in Fig. 6 a (with circles) for E = 600 eV were obtained.

The trend of the potential shown in Fig. 8 can also be approximated by the function $V = 3.55/r^4$. Also presented in this same figure is the trend of $^2\Pi$ and ^2Z terms of the system Ne^+-He calculated in [3]. From the figure it is clear that the intersection of the $^3\Sigma$ term with the cutoff of the continuous spectrum can occur only in the region of very strong approach ($r < 1$ Å), not attainable for the range of scattering angles examined here. This last statement is valid only insofar as the /11

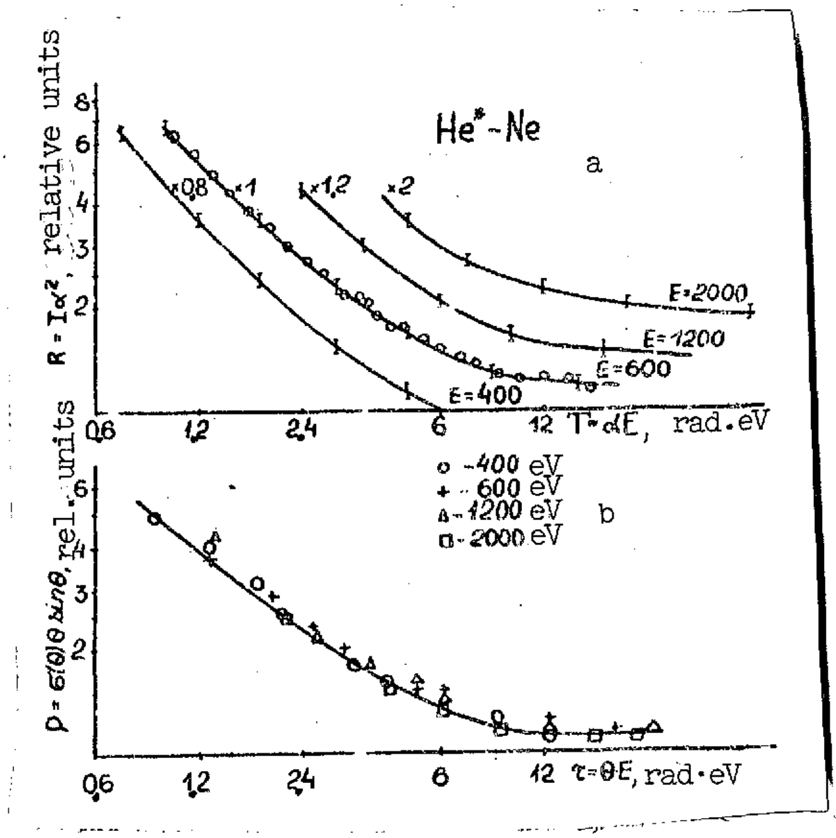

Fig. 6. Experimental functions R(T) for the system He*-Ne (a) and a single function ρ (r)(δ) derived therefrom

calculations of the terms $^2\Sigma$ and $^2\Pi$ are valid. To verify the accuracy of these calculations, measurements were made of scattering in helium of a 400 eV Ne^+ beam. Fig. 7 presents the measured (solid line) curve of R(T) and the R(T) curve calculated on the basis of the theoretical potentials given in [3]. From the figure it is clear that the calculated function differs very strongly from the experimental function and that this discrepancy indicates imprecision in the calculations given in [3].

The monotonicity of $^2\Sigma$ and $^2\Pi$ potentials does not permit determining their trend by combining the current calculated from the varied potentials with the experimental current. In this case, it is possible to restore only the effective term.

Conclusion

1. Measurements were made of the differential scattering of the systems He*-He, He*-Ne, and Ne*-He.

2. The experimental functions obtained were compared with the functions calculated from known literature data on the interaction potentials of the systems He*-He and Ne*-He. Discrepancies

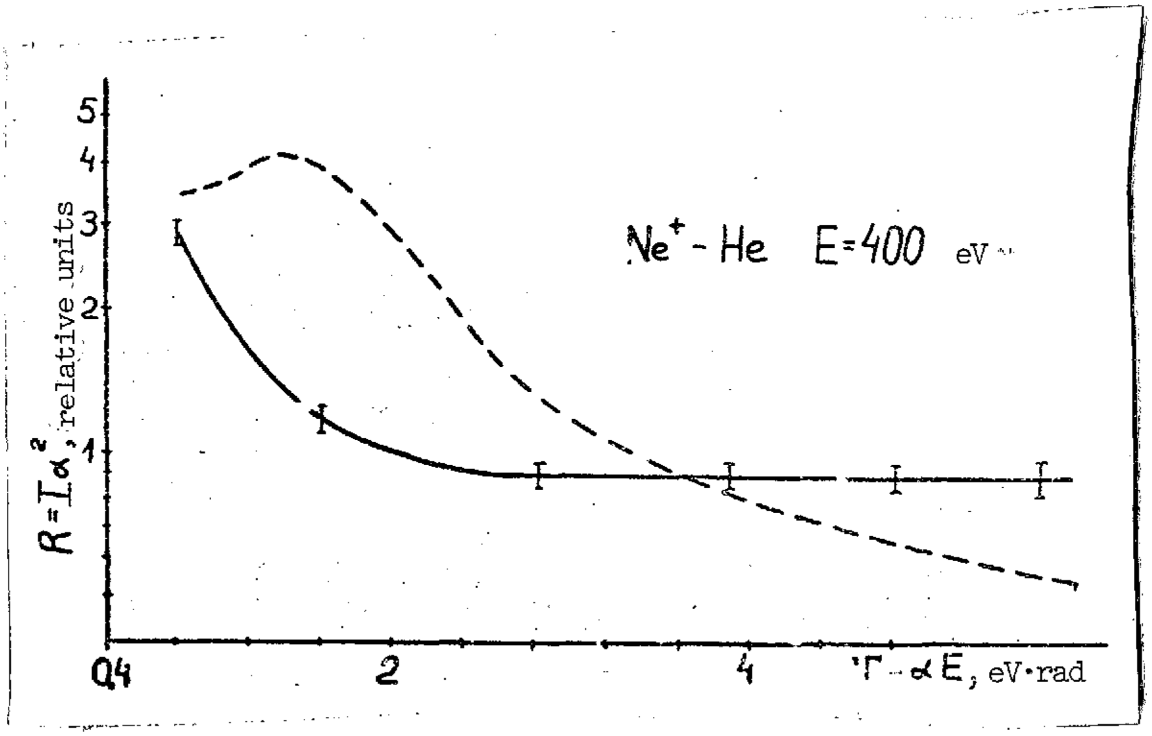

Fig. 7. Comparison of experimental function R(T) and R(T) calculated according to [3]

were found and the methods of eliminating them are discussed.

3. The function of the potential energy corresponding to the term $^3\Sigma_g^+$ of the system He_2 was found and its analytical approximation was proposed.

4. For the system He*-Ne, the conversion of the experimental functions $I(\sigma)$ into differential scattering cross-sections showed the absence of interaction with the continuous spectrum in the region of the approach distances investigated; the dependence of V(r) for the system He*-Ne was found for the range of n values from 0.7 to 2.5 Å.

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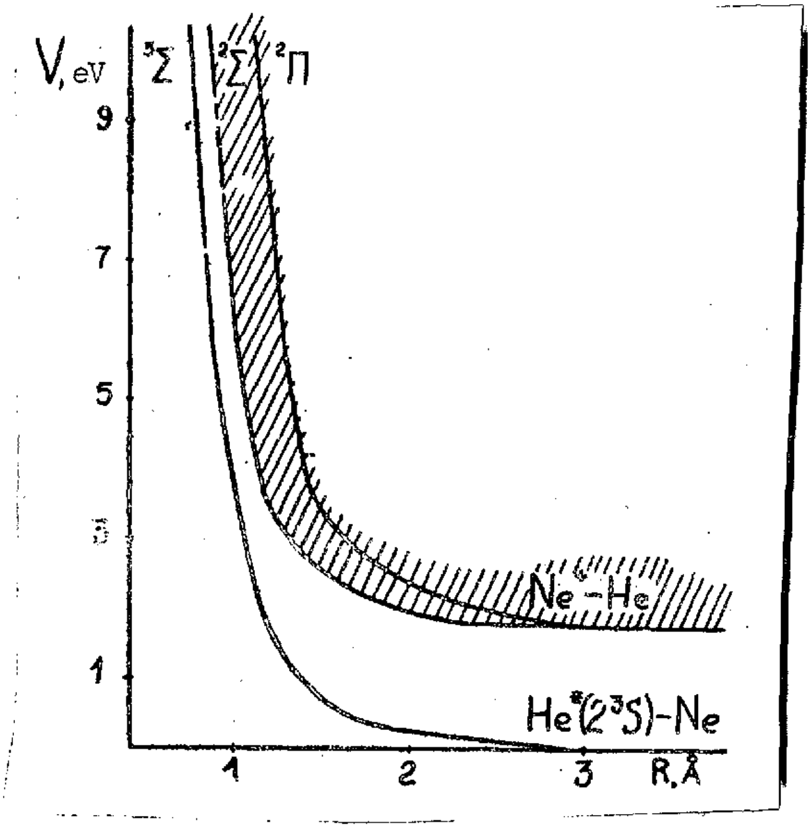

Fig. 8. Trend of the potential of the system Ne-He found in the present study and its approximation with the terms $^2\Pi$, $^2\Sigma$ of [3]

REFERENCES

1. Smirnov, B. M., Asimptoticheskiye metody v teorii atomnykh stolknoveniy /Asymptotic methods in the theory of atomic collisions/, Moscow, Atomizdat, 1972. /12
2. Duman, Ye. L., Tezisy konferentsii po fizike elektronnykh i atomnykh stolknoveniy /Abstracts of Papers Presented at the Conference on Electronic and Atomic Collisions/, Riga, Znaniye Press, 1969, p. 141.
3. Kalinin, A. P., Leonas, V. B., and Sermyagin, A. V., Vestnik MGU, series 3, 3, 245 (1971).
4. Mott, G., and Messi, G., Teoriya atomnykh stolknoveniy /Theory of atomic collisions/, Mir Press, 1969.
5. Kolker, H. J., and Michels, H. H., J. Chem. Phys., 50, 1763 (1969).
6. Michels, H. H., and Harris, F. E., J. Quant. Chem. 25, 51 (1968).
7. Layton, J. K., J. Chem. Phys., 59, 5744 (1973).
8. Peterson, J. R., and Lorents, D. C., Phys. Rev. 182, 152 (1969).
9. Morgenstern, R. et al., Phys. Rev. 8A, 2372 (1973).
10. Olson, R. E., and Smith, F. T., Phys. Rev. 7A, 1529 (1973).
11. Smith, F. J., Physica, 30, 497 (1964).
12. Ginter, M. L., and Battino, R., J. Chem. Phys. 52, 4469 (1970).
13. Sandro, K. M., Mol. Phys. 23, 413 (1972).
14. Evans, S. A., Cohen, J. S., and Lane, N. F., Phys. Rev. 4A, 2235 (1971).